Energy Transfer in O Collisions with He Isotopes and Helium Escape from Mars

Energy transfer in O collisions with He isotopes and Helium escape from Mars

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[1] Accurate data on energy-transfer collisions between hot oxygen atoms and the atmospheric helium gas on Mars, are reported. Anisotropic cross sections for elastic collisions of $O(^3P)$ and $O(^1D)$ atoms with helium gas have been calculated quantum mechanically and found to be surprisingly similar. Cross sections, computed for collisions with both helium isotopes, ^{3}He and ^{4}He, have been used to construct the kernel of the Boltzmann equation describing the energy relaxation of hot oxygen atoms. Computed rates of energy transfer in O+He collisions have been used to evaluate the flux of He atoms escaping from the Mars atmosphere. Atmospheric layers mostly responsible for production of the He escape flux are identified. Our results demonstrate that strong angular anisotropy of scattering cross sections increases the collisional ejection of light atoms and is critical in the evaluation of He escape from Mars, Venus and Earth. **Citation:** Bovino, S., P. Zhang, F. A. Gianturco, A. Dalgarno, and V. Kharchenko (2011), Energy transfer in O collisions with He isotopes and Helium escape from Mars, *Geophys. Res. Lett.*, *38*, L02203, doi:10.1029/2010GL045763.

1. Introduction

[2] Helium is one of the dominant constituents in the upper atmospheres of Mars and Venus [*Krasnopolsky and Gladstone*, 2005; *Krasnopolsky et al.*, 1993]. Helium escape is crucial for understanding the evolution of the Martian atmosphere and modeling elemental abundances in the Mars interior [*Krasnopolsky and Gladstone*, 1996; *Barabash et al.*, 1995]. Information on the He balance in the upper atmosphere is also important for analysis of the degassing history of the planet as well as the interaction between the solar wind and the Martian exosphere [*Barabash et al.*, 1995; *Chanteur et al.*, 2009]. Since Mars has a negligible intrinsic magnetic field [*Acuña*, 1998], the solar wind can penetrate deeply into the neutral corona. This process contributes to a global erosion of the atmosphere but also provides additional He atoms due to neutralization of α-particles. The thermal escape of He is negligible on Mars [*Chassefiére and Leblanc*, 2004] and the major mechanism of escape is the collisional ejection of He atoms by energetic oxygen. This process turns out to dominate over ion-related mechanisms, such as sputtering by pick-up ions [*Krasnopolsky*, 2010]. To obtain an accurate evaluation of the escape flux of neutral He becomes a fundamental issue. In this letter, we investigate the collisional ejection of He atoms by energetic O atoms, produced in the dissociative recombination of O_2^+ ions [*Ip*, 1990; *Fox*, 1993; *Kim et al.*, 1998; *Hodges*, 2000]. The rate of production of energetic oxygen atoms varies with solar activity [*Fox et al.*, 1996]. We report below the results of an accurate evaluation of the energy transfer from hot O (^{3}P, ^{1}D) atoms to the atmospheric He gas. We have calculated angular dependent cross sections for collisions of hot O (^{3}P,^{1}D) atoms with the thermal ^{4}He and ^{3}He atoms and constructed the kernel of the Boltzmann equation, which describes the rate of energy transfer collisions. Energy distribution functions of the He recoil atoms have been computed at different altitudes and the He loss rate is evaluated for the Martian upper atmosphere at low solar activity.

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2. Quantum Cross Sections and Energy Transfer in O+He Collisions

[3] The correct description of the relaxation kinetics of energetic atoms in dilute atomic bath gases requires detailed information on the interaction potential and the collision cross sections. We begin our study with an accurate quantum-mechanical determination of the interaction potentials of He atoms with $O(^3P)$ and $O(^1D)$ atoms. Multireference configuration interaction [*Werner and Knowles*, 1988] and coupled cluster [*Knowles et al.*, 1993] methods were used to calculate the potential energy curves for $O(^3P)$+He and $O(^1D)$+He; the final potentials have been further extrapolated to the complete basis set limit [*Varandas*, 2007]. Differential cross sections of elastic collisions have been calculated by solving the Schrödinger equation for each individual electronic potential curve. The final cross sections are obtained from the statistically weighted sum of the individual molecular channels. For $O(^1D)$, the three potentials are $^1\Sigma$, $^1\Pi$, $^1\Delta$ with statistical weights 1/5, 2/5 and 2/5 respectively. For $O(^3P)$, they are $^3\Pi$, $^3\Sigma$ with weights 2/3 and 1/3. Computed total and diffusion cross sections [*Zhang et al.*, 2009] are shown in Figure 1 for both He isotopes. Interestingly, the cross sections for $O(^3P)$ and $O(^1D)$ show a very similar energy dependence with small differences appearing only in the high energy region, where scattering is dominated by the repulsive part of the interaction potential. The differences between the cross sections of the isotopes ^{3}He and ^{4}He colliding with oxygen are also small and become relatively large only at very low collision energies (<0.005 eV). With quantum mechanically calculated differential cross sections, we have constructed the kernel of the Boltzmann equation $B(E'|E)$ which describes the rate of transition from initial kinetic energy E' to final energy E in the laboratory frame (LF) [*Kharchenko et al.*, 1997, 1998, 2000; *Zhang et al.*, 2008]. The temperature (T = 220 K) used in the kernel calculations corresponds to conditions of the upper

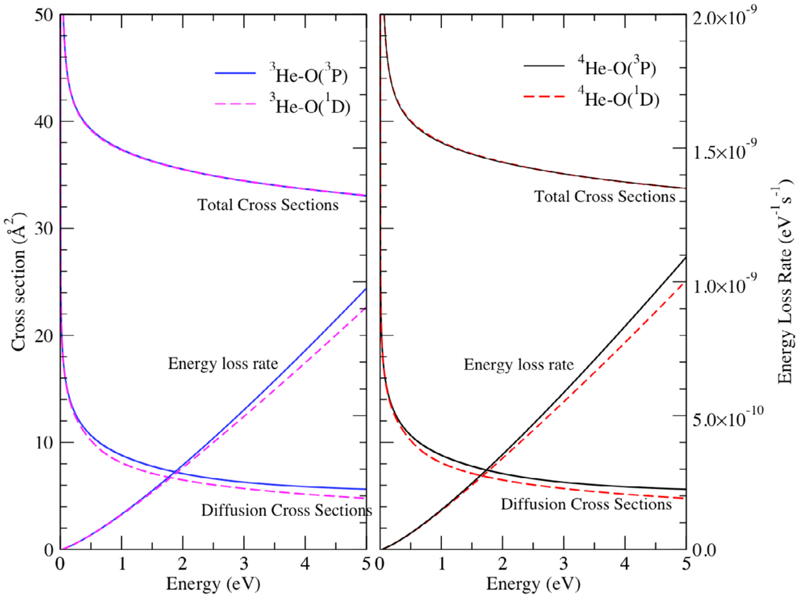

Figure 1. Total and diffusion cross sections of O(^{3}P)–^{4}He. (solid lines) and O(^{1}D)$^{-4}$He (dashed lines) collisions as functions of center of mass scattering energies. For energy loss rates $\gamma(E, T)$ the horizontal axis represents the initial energy in laboratory frame. The total cross sections of O(^{3}P)-He and O(^{1}D)-He are so close that the two curves overlap.

atmosphere of Mars at an altitude of 250 km. According to *Krasnopolsky and Gladstone* [2005], it remains practically constant up to 400 km. The energy loss rate $\gamma(E, T)$, computed for unit bath gas density, of hot O atoms $\gamma(E, T) = \int B(E'|E)(E - E')dE'$ is shown in Figure 1 as a function of the initial LF energy. For both O(^{1}D) and O(^{3}P) the energy loss rates increase with the initial LF energy by an amount equal to the difference in the diffusion cross sections.

3. Escape Flux of the He Atoms

[4] Distributions of the secondary hot atoms produced in recoil collisions with energetic oxygen are crucial for the determination of the escape flux of the He atoms from terrestrial planets. The escape energies (E_{esc}) of ^{4}He and ^{3}He in the Martian atmosphere are 0.48 eV and 0.36 eV respectively. If the recoil atoms gain enough energy in the upward direction, they could escape from the atmosphere. Reliable estimates of the He escape flux can be made using the Boltzmann kernel, which yields information on O+He recoil collisions and provides the fraction of the secondary hot atoms with energies E_r larger than the escape energy E_{esc}. The energy distribution function $\rho(E_r|E)$of recoil atoms, normalized to unity, is given by $\rho(E_r|E) = B(E - E_r|E)/\int B(E'|E)dE'$. Distributions calculated at selected initial energies E_i are shown

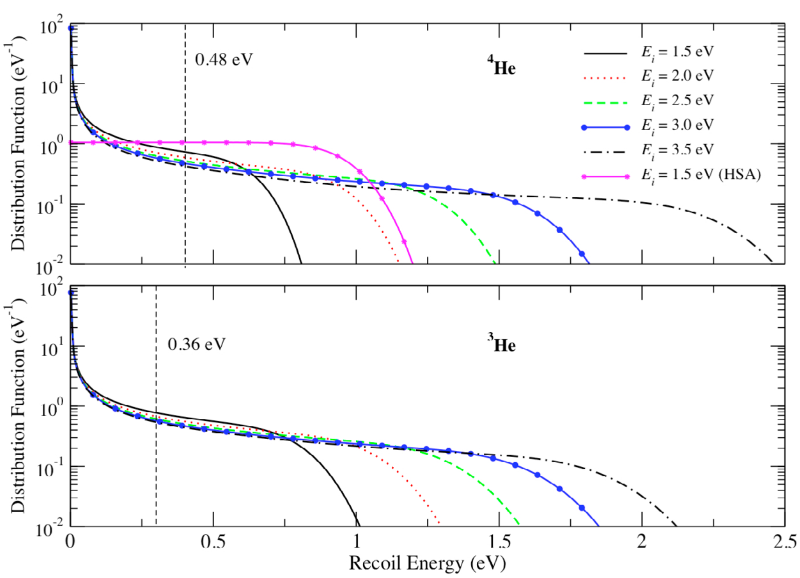

Figure 2. Distribution functions of secondary fast atoms as functions of recoil energy for O thermalized in ^{4}He or ^{3}He bath gases at selected initial laboratory frame energies. The vertical dashed lines indicate the escape energies of ^{4}He and ^{3}He (0.48 and 0.36 eV) from the Martian atmosphere.

Table 1. Percentage of the Secondary Energetic ^{4}He and ^{3}He Atoms Capable of Escaping Produced by Hot O(^{3}P) and O(^{1}D)

	% O(^{3}P)		% O(^{1}D)	
E_i(eV)	^{3}He	^{4}He	^{3}He	^{4}He
1.0	14	10	13	9
1.5	23	20	23	19
2.0	29	25	28	24
2.5	32	29	31	27
3.0	34	31	33	29
4.0	37	34	35	32

in Figure 2. The vertical dashed lines in Figure 2 indicate the escape energy of the atomic He from the Martian atmosphere. The percentage of the recoil ^{4}He and ^{3}He, generated by both O(^{3}P) and O(^{1}D), with energies above the escape energy threshold can be calculated as

$$\Gamma(E_i) = \int_{E_{esc}}^{\infty} \rho(E_r|E_i)dE_r. \quad (1)$$

The results are listed in Table 1 for the selected E_i. The fraction of secondary hot atoms increases with the initial projectile energy. The results clearly show that the O(^{3}P) and O(^{1}D) relaxation kinetics are similar, and the related percentage of hot He agrees within 2%. It is possible therefore to treat them in escape modeling as single oxygen particles. For comparison, the distribution of ^{4}He atoms produced in the recoil collisions with hot O atoms is calculated with the Hard-Sphere approximation (HSA). The results are depicted in Figure 2 for the oxygen initial energy E_i = 1.5 eV. The percentage of the recoil ^{4}He with energies above E_{esc} is 49%, which is 2.5 times larger than the 19% obtained from the angular-dependent differential cross section.

[5] O_2^+ is the major molecular ion in the upper atmosphere of Mars [*Fox*, 1993], and it is the main source of hot oxygen atoms. The quenching of O(^{1}D) to O(^{3}P) in collisions with thermal He may be neglected because of the small rate constant [*Heider and Husain*, 1974]. In our simplified approach, the rate of production of hot O atoms at the altitude h with initial energy E_i, $f(E_i, h)$, has been constructed considering the four dissociation channels with the exothermicities and branching ratios of the ground vibrational state compiled by *Kella et al.* [1997], *Petrignani et al.* [2005], and *Guberman* [1988]. The distributions of the nascent O have been constructed analytically by transforming the initial energy distributions from the center of mass (CM) to LF [*Forrey et al.*, 1996]. We considered the conditions of low solar activity with the nascent hot O distributions corresponding to the atmospheric production rates below 400 km from *Fox and Hać* [2009]. Above 400 km, we adopted the atmospheric model by *Krasnopolsky and Gladstone* [1996], and obtained the altitude-decreasing weak source of hot O by extrapolation [*Fox and Hać*, 2009]. We restrict our further attention to ^{4}He.

[6] For the simplified one-dimensional atmospheric model, the altitude yield of hot helium atoms, moving upwards with energy exceeding E_{esc}, is given by:

$$P(h_1) = \frac{1}{2}\int_0^{\infty} dE_i T_1(h_1, E_i) n_1(h_1)\Gamma(E_i)\sigma_{12}^{eff}(E_i) \cdot \int_{h_2^{min}}^{h_1} dh_2 f(E_i, h_2) T_2(h_2, h_1, E_i) \quad (2)$$

where the index 1 and 2 refers to He and O atoms respectively; the expression $n_1(h_1)\Gamma(E_i)\sigma_{12}^{eff}(E_i)$ is the inverse of the mean free path for O+He collisions in which the energy transfer is above the escape threshold, and the transparency factor T_2

$$T_2(h_2, h_1, E_i) = \exp\left[-\int_{h_2}^{h_1} dh' \sum_j \sigma_{j2}^{eff}(E_i) n_j(h')\right] \quad (3)$$

is the probability for hot oxygen atoms, produced at the altitude h_2, to reach the altitude h_1 without energy-loss collisions. T_2 describes the energy-relaxation process in the upward moving flux of fast oxygen atoms and effective cross-sections σ_{j2}^{eff} have been determined from the analysis of experimental data or results of the numerical solutions of the Boltzmann kinetic equation for thermalization of hot O in atmospheric gases [*Kharchenko et al.*, 1997; *Takahashi et al.*, 2002; *Balakrishnan et al.*, 1998, 1999; *Zhang et al.*, 2009].

[7] The summation in the exponential includes the major constituents of the Martian upper atmosphere, CO_2, CO, N_2, O_2, H_2, H, Ar, and He. We found that energy relaxation cross sections are close to averaged values of diffusion cross sections and we have used diffusion cross sections in our evaluation of the transparency factor T_2. The corresponding cross sections for N_2-O, O_2-O and O-H were taken from *Kharchenko et al.* [2000], *Balakrishnan et al.* [1998], *Brunetti et al.* [1981], and *Zhang et al.* [2009] respectively. Since no data for collisions of atomic oxygen with CO_2 and CO molecules are available, we approximated these cross sections by those of O-O_2 and O-N_2 respectively. Similarly, O-H_2 collisions were approximated by O-N_2. For further simplification, O-O collisions are not included in the energy relaxation scheme for nascent hot O, because these collisions do not reduce the total kinetic energy of hot O, if energetic recoil O atoms are included in the upward flux of hot atoms. The other transparency factor T_1 in equation (2),

$$T_1(h_1, E_i) = \exp\left[-\int_{h_1}^{h_1^{max}} dh' \sum_j \sigma_{j1}^{eff}(E_i) n_j(h')\right], \quad (4)$$

is the escape probability of energetic He atoms produced in collisions with hot O. The summation in equation (4) is similar to that of equation (3) except that the thermal He is not included. In our calculation, $h_2^{\min}$ is chosen to be 130 km, and $h_1^{\max}$ = 700 km. The altitude yield of escaping He atoms, $P(h_1)$, calculated from equation (2), is shown in Figure 3 for low solar activity conditions. The solid curve shows results of our calculations with the diffusion cross sections defined earlier. To illustrate the sensitivity of the He escape flux to collision cross sections, $P(h_1)$ has been computed by replacing in the transparency factors T_2 and T_1 the diffusion cross sections with the total cross sections. Results are shown in Figure 3 by the dashed curve. While the total cross sections accurately represent a collisional depth, they do not account properly for the energy relaxation in the upward O flux and they underestimate the contribution of energetic O atoms. Accurate treatment of this energy relaxation is especially important in the region of efficient production of hot O atoms (150–200 km), which has been neglected in the exobase

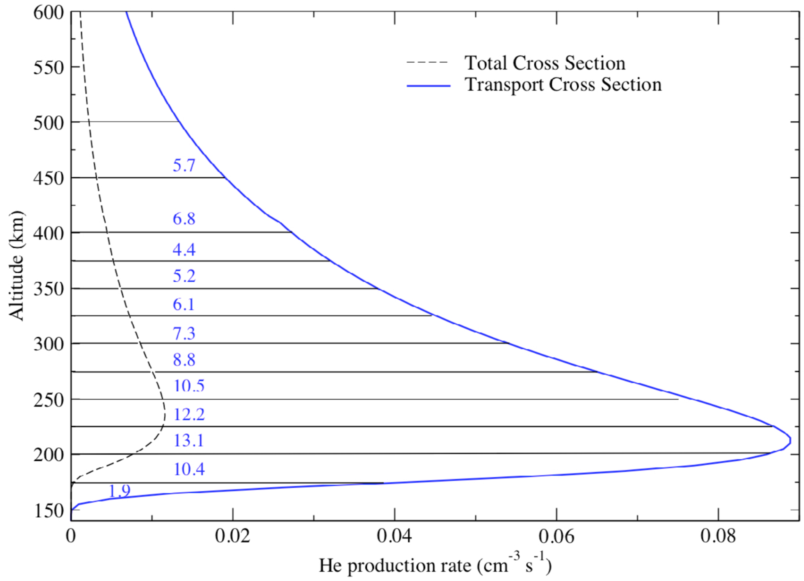

Figure 3. The production rate of ^{4}He escape flux as a function of altitude. Dashed and solid lines represent results evaluated using total cross-section and transport cross-section respectively. Numbers in Figure 3 represent the percentage contribution from each atmospheric layer.

approximation. These atoms collide with the atmospheric gas and lose only small fraction of their initial energy but contribute significantly to the collisional ejection of He atoms below and above the exobase level of 200 km. The yield of escaping He has a maximum around 230 km.

[8] The He column escape flux F^{esc} is obtained by integrating the production rates over all altitudes considered (130–700 km), $F^{esc} = \int_{130}^{700} dh_1\, P(h_1)$. The percentage contribution to the column escape flux from each atmospheric layer of 25 km height is shown in Figure 3. The greatest contribution comes from the layer ranging from 170–400 km, and the yield of escaping He from altitudes lower than 200 km is considerable. The computed column rate of He escape flux for the day side of the Mars atmosphere is $F^{esc} = 1.7 \times 10^6$ cm^{-2} s^{-1} at the minimum of the solar activity. This value is in close agreement with an estimate of the He escape flux, 1.6×10^6 cm^{-2} s^{-1}, obtained from the reported rates of oxygen escape fluxes [*Fox and Hać*, 2009, 2010], the cross section of O+He collisions, and the averaged value of the escape fraction $\langle \Gamma(E_i) \rangle$. The column rate of the He escape rate computed with the total cross sections is seven time smaller, because it strongly suppresses the escape fluxes from the regions below the exobases of 200 km. We computed the rate of nonthermal losses Q of the atomic He from the upper atmosphere of Mars as $Q = F^{esc} S_{\max}$, where $S_{\max} = 2\pi\,(h_1^{\max} + R_M)^2$ is the area of the illuminated Martian hemisphere at $h_1^{\max}$ and R_M is the volumetric mean radius.

[9] The result obtained considering both O(^{3}P) and O(^{1}D), for $h_1^{\max} = 700$ km is 8.9×10^{23} s^{-1}, which is almost twice the escape rate computed in the exobase approximation by *Krasnopolsky and Gladstone* [2005] (5×10^{23} s^{-1}). This order of magnitude agreement could be considered as accidental: the atmospheric, the ionospheric, and collision parameters are different in these two models, and the exobase approximation does not consider the atmospheric regions below 200 km, which are important for production of hot O and He escape fluxes. Strong angular anisotropy of collision cross sections yields a result differing several times with the HSA calculations [*Krestyanikova and Shematovich*, 2006; *Fox and Hać*, 2009, 2010; *Zhang et al.*, 2009].

[10] The knowledge of the accurate angular dependent cross sections is fundamentally important for the determination of the upward fluxes of energetic atoms. The degradation of upward atomic fluxes in the simplified modeling may be computed with the effective hard sphere cross sections, describing the energy relaxation process, or with related diffusion cross sections. Value of the effective hard sphere cross section can be determined only by fitting accurate data on the energy relaxation obtained in laboratory experiments, the solutions of the Boltzmann kinetic equation, or Monte Carlo simulations of the thermalization process.

4. Conclusions

[11] Collisional kinetics and transport properties of energetic oxygen atoms in collisions with ^{3}He and ^{4}He have been determined. Accurate interaction potentials have been calculated for O(^{3}P) and O(^{1}D) atoms interacting with He and employed to obtain total, diffusion, and differential cross sections. The latter have been used to construct the kernel of the Boltzmann equation and evaluate the energy loss rate. Distributions of energetic helium atoms, produced in O+He recoil collisions in the upper atmosphere of Mars, have been investigated. The production rate and escape flux for ^{4}He have been calculated and the contributions from different atmospheric layers to the He escape flux have been determined. The total loss of helium due to the collisions with hot oxygen atoms produced by dissociative recombination of O_2^+ was evaluated and compared with previously reported results. The computed He escape flux agrees closely with the estimate based on the reported values of the Martian oxygen escape flux [*Fox and Hać*, 2009, 2010]. The escape flux depends strongly on the altitude distribution of O_2^+ ions and undergoes significant time and spatial variations.

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